

T DIVISION CONTRIBUTIONS TO APPENDIX F MEASURES

Performance Objective #1: Conduct warhead certification and assessment actions using a common UC Design Laboratory Strategy.

T Division plays a central role in developing high-fidelity physics models to enhance the predictive capabilities of the simulation tools used by the warhead certification and assessment community. The Advanced Simulation and Computing (ASC) program's Materials and Physics (M&P) program element at Los Alamos supports the majority of these physics enhancements, and T Division is the single largest contributor to that program. These improvements are evaluated through the Quantification of Margins and Uncertainties (QMU) framework, which has been developed in a joint UC/ LANL/LLNL process.

Performance Objective #2: Develop with NNSA and implement long-term, balanced, integrated stewardship.

(Performance Measure) PM 2.1. Support the needs of warhead assessment, certification, and simulation validation by executing a coordinated program of targeted small- and large-scale experiments and mining of archival UGT data to improve predictive capability. Develop and execute a program of hydrotests and subcritical experiments that addresses assessment and certification needs.

In conjunction with our responsibilities for weapons physics theory and model development, the Division Principal Investigators (PIs) and staff work with our experimental colleagues to ensure that the data necessary for validation purposes are obtained and that the program plans of the Experimental Physics Program are coordinated with those of the Theoretical and Computational Programs. In this way the fundamental validation process can be performed with the relevant small-scale ("single physics") experimental data. Once the models are implemented into the simulation codes they can be further validated against the integral ("multi-physics") data from hydrotests, subcritical, and other large-scale experiments. The ASC M&P program is organized into a suite of constituent projects representing relevant discipline areas (e.g., equation of state, atomic physics, nuclear physics) that correlate to the Division's group structure. The individual PIs and their group management interact with the various project leaders and program managers to perform this coordination.

The contributions of T Division to modeling and theory for the weapons programs can be more fully appreciated by examining the specialties of each of the groups as described in the Organizational Summary (see pages 4-8), as well as in the research papers and other quantitative measures of accomplishment provided throughout this document. T Division has also had responsibility for managing the Laboratory-wide ASC M&P Modeling project up until December 2004 when a reorganization consolidated all Laboratory weapons program managers into the newly created Principal Associate Directorate for Nuclear Weapons Programs.

PM 2.2. Conduct design and analysis of nuclear weapons that address the future needs of the US nuclear deterrent.

T Division has a supporting role in the area of weapons design and analysis. Our role is one of consulting with the assessment community as subject matter experts of the underlying physics, as that physics is expressed in the simulation tools. In this way we identify the shortcomings of the currently implemented physics and can then work to target and develop enhanced, physics-based models for future implementations, creating evermore-predictive tools for the assessors.

PM 2.4. Develop and demonstrate ASC simulation and modeling capabilities that support the ongoing needs of stockpile assessment and certification.

Certification or assessment plans for more than one of the Laboratory's weapons systems are explicitly linked to milestone deliveries from T Division. This represents a significant change from even the recent past. In addition, the Division has played a central role in the formulation of the methodology for quantification of margins and uncertainty (QMU) and the implementation of the Laboratory Strategic Goal A (Science-Based Prediction). Assessing our evolving predictive simulation capability also requires significant efforts in validation and verification, especially uncertainty quantification (UQ). T Division is also a member of the "G4," an advisory body to the Program Director of the ASC Program, comprised of the four division offices that execute the majority of the Program (X, T, CCS, and CCN). As a result, T Division plays a significant role in planning the Program's future.

Among the principal issues of stewardship vigorously addressed is predictability and uncertainty quantification. This requires an extensive knowledge of equations of state, material strength, nuclear cross sections, opacities, and the chemistry and material science of aging. T Division remains the principal Laboratory focus for the theoretical foundations of these properties. A broad set of knowledge of material dynamics is required. This includes the effects of strength, failure, spall, instability, turbulence and mix, and the Division continues a long-standing position of preeminence in the theory, modeling, and simulation of these processes, as well as providing guidance for the performance of experiments necessary to gather relevant additional data.

Improved predictability requires powerful numerical techniques for the complex dynamics in a weapon environment. Among the Division's staff are world leaders in code development and applications. Our computational codes incorporate the best physical data and motivated models for material instability mix, turbulence, radiation transport, and nuclear and chemical transitions. They are robust and efficient even in the presence of a strong distortion of interacting materials driven by large concentrations of rapidly released energy. In recent years, the computer codes have been ported to new, highly parallel machines.

PM 2.5. Improve and apply tools and models for prediction of systems, subsystems, and/or component lifetimes.

The aging nuclear stockpile requires continual maintenance, and surveillance of the stockpile will continue to reveal a host of aging issues. The expertise and experience within the Division allows us to remain active on several fronts to ensure that the stockpile remains reliable and that safety is not compromised. New opportunities to support the Stockpile Stewardship Program include uncertainty quantification, polymers and high explosives, equations-of-state, opacities, nuclear cross-sections, high energy-density physics, and nonequilibrium phenomena.

PM 2.6. Develop and implement a collaborative and complementary program of experiments at High Energy-Density (HED) facilities that supports assessment and certification needs.

Division personnel are active participants in collaborations involving HED facilities that support assessment and certification needs. Research in areas ranging from fast-particle stopping in warm dense matter, equations of state of HED matter, and x-ray Thomson scattering diagnostics for dense plasma diagnosis are currently underway. Many of the experiments are currently being carried out at the Trident laser facility, with smaller-scale laser-based experiments also in progress. T Division activities are supported through the Boost program (C1), Thermonuclear Burn Project (ASC), and LDRD.

PM 2.7. Develop and implement an integrated program with a central goal to achieve ignition at NIF in 2010.

Through the work performed in T Division in the areas of atomic physics (including opacities) and thermonuclear burn (important elements of the ASC M&P portfolio), our work improves the ability of the Laboratory to contribute to this important national goal. In addition, we have Division staff supported directly under Campaign 10 (Ignition) working directly with the Experimental Program on ignition issues at NIF.

PM 2.8. Develop and implement an integrated program for plutonium capabilities of LANL and LLNL to support the overall NNSA strategic requirements.

Personnel from T Division, including the Equation of State Project Leader, the M&P Program Manager, the Pit Lifetimes PI, and senior staff, have all been directly involved in several recent workshops and reviews of the plutonium capabilities at LANL. These meetings have worked to develop a consensus tri-lab evaluation of the current capabilities, and a program plan for modeling and data needs. This has served as a basis for discussions about the facilities required to obtain the data necessary to guide and validate model improvements.

Performance Objective #3: Develop with NNSA and implement near-term balanced weapon programs that are coordinated with the other NNSA Management and Operations (M&O) site contractors and DoD customers and that foster complex-wide solutions to meet the needs of the US nuclear deterrent.

PM 3.1. Conduct stockpile surveillance activities, investigate significant findings and issues identified in technical assessment reports on a prioritized basis, and establish closure plans for Significant Finding Investigations (SFIs).

T Division has an increasingly large portfolio in the surveillance program. In addition to the significant contributions we have made in the areas of high explosive and canned subassembly (CSA) lifetimes, the T-1 Group Leader now serves as the lead PI on the Laboratory's pit lifetimes equation of state effort. Work from T Division has been directly used as part of SFI closures and more work has been commissioned for future SFI issues.

PM 3.2. Deliver on the major milestones for the Life Extension Programs for the W76, the B61-7/11, and the W80-3 in accordance with the joint DOE/DoD phase 6.x process.

T Division is supporting these programs by helping to identify critical aging components through various collaborative projects.

PM 3.3. Deliver on W88 Pit Manufacturing and Certification Project major milestones.

T Division has contributed to understanding major material and fabrication issues that are crucial to the successful execution of the W88 pit manufacturing at Los Alamos. Simulation tools for the W88 Pit casting have been enhanced by contributions from Division personnel. The W88 certification plan specifically calls out contributions from T Division. This work is currently underway.

PM 3.4. *Meet directive schedule requirements.*

All Laboratory Nuclear Weapons Programs work is planned using project management tools and standards. T Division is subject to all relevant components of that schedule for its specific deliverables.

PM 3.6. Complete the establishment of, and implement in accordance with NNSA-approved plans, a weapons design and manufacturing quality assurance program consistent with NNSA requirements.

Beginning this year with Revision 10, the QC-1 Quality Control plan for the weapons program, includes within its scope R&D activity, whereas in previous years this only included facilities and manufacturing. As a result the weaponssupported work in T Division is subject to certain standards of quality assessment. In the graded approach being adopted, the longer-term research primarily done in the Division relies significantly on the academic peer-review process. A recent audit found no issues in T Division.

PM 3.7. Develop and execute projects to improve the responsiveness of the design, manufacturing, and testing infrastructure of the integrated nuclear weapons complex.

The increasingly predictive simulation tools to which we contribute significantly will, over time, result in a more efficient and less costly means of performing our stockpile stewardship mission. While we will always conduct small- and largescale experiments in support of our mission, we should become less reliant on them, answering a greater fraction of questions that arise by means of our validated simulation tools.

Performance Objective #4: Implement an integrated science and technology-based program aimed at preventing the proliferation or terrorist acquisition of weapons of mass destruction as well as detecting and responding to their deployment or use.

PM 4.1. Provide technical capabilities to limit or prevent the spread of materials, technology, and expertise relating to weapons of mass destruction; eliminate or secure inventories of surplus materials and infrastructure usable for nuclear weapons; and enable the implementation of US nonproliferation policy.

The Division is making significant contributions to the detection of nuclear materials by drawing on our capabilities in nuclear physics to aid in detector design and analysis. This has proved useful in support of both securing materials in this country and abroad and in monitoring borders against the covert introduction of nuclear materials. We have also

played a role in quantifying the utility of nontraditional nuclear materials for weapons use and in working with the design community to anticipate possible improvised nuclear device (IND) designs. Knowledge of alternative IND designs is an important prerequisite to looking for signs of proliferation and for assessing our vulnerability to terrorist attack.

Exciting new initiatives in the area of biological weapons and attacks are discussed in PM 4.4.

PM 4.2. Provide scientific research capability that produces cutting-edge R&D as well as the testing and evaluation needed to detect, identify, and monitor proliferation and terrorist-related weapons of mass destruction activities.

As a strong technical division involved in research, T Division is a significant resource for the Laboratory as it moves to increase its business in Threat Reduction activities—a strategic direction for Los Alamos. Drawing on our strengths in multidisciplinary research in theory, modeling, and simulation, the Division brings significant capabilities to these emerging needs. Our substantially enhanced strategic partnering with the Laboratory's Threat Reduction Directorate and the CHS is in the clear interests of the Division, the Threat Reduction programs, and the Laboratory.

PM 4.3. Support the needs of the intelligence community by providing intelligence analysis capabilities and science and technology that improve the nation's ability to detect and thwart proliferation and terrorism.

In addition to the consulting on matters of nuclear weapons technology that T Division members have done traditionally, several new areas of support of the Intelligence Community (IC) have emerged in T Division over the past few years and have resulted in a clear growth area for the Division. We have multiple sponsors currently in place for analyses of terrorist networks and their capabilities using agent-based modeling methods. In addition, Division staff are working at the forefront of fundamental discoveries of networks and their behavior, which are beginning to find application in such diverse areas as infrastructure vulnerability analysis (e.g., power grid), communication network optimization, and spread of biological epidemics. The Division's capabilities in nuclear physics are proving very important in developing the means of analyzing the debris in the aftermath of a nuclear device detonated by a terrorist to determine the source of the material, hence identifying its origin. This "attribution" effort draws from capabilities developed under sponsorship of the nuclear weapons program to meet new threat reduction missions, and is currently funded from NNSA. We are also finding applications for our capabilities in the analysis of very large-scale data sets to identify patterns, connections, and hidden signals in the extremely large bodies of data collected by the IC. Our materials capabilities are likewise finding sponsorship in support of intelligence needs, including design of novel sensors and detectors, and in predicting the behavior of "designer materials" not yet synthesized. Finally, there are significant new programmatic opportunities for our exceptional strengths in the biological arena as described in PM 4.4.

PM 4.4. Develop and support the deployment of technologies and analytical capabilities that strengthen the Nation's ability to protect against and respond to terrorist use of weapons of mass destruction and other threats against the US homeland.

T Division has taken leadership over the past years in championing the broader application of predictive science, including uncertainty quantification, in mission areas beyond NW programs. This activity led to the successful development of two multidivisional projects that not only address homeland security needs, but also are providing a vision and path forward for the biosciences at the Laboratory.

The first project is in support of the DHS's Science and Technology Office of Research and Development in the area of biological threat characterization and analysis for the National Biodefense and Countermeasure Analysis Center (NBACC). At the sponsor's request, a T Division-lead project was initiated in August 2004 to develop a methodology to provide the Nation's first biological risk assessment that is transparent and defensible, in response to the Homeland Security Presidential Directive 10 (HSPD-10). The deliverable for the measure is to:

develop a suite of methodologies for the generation of the first-pass risk assessment in support of the NBACC, amenable to regular (e.g., biannual) and immediate updating. Use this methodology to complete a preliminary risk assessment of classical biological threats.

The multidivisional team developed the methodology, applied the tool, and provided the above deliverable on time in January 2005. Upon assessment of the preliminary project, the sponsor is continuing the effort for an October 2005 deliverable funded at \$7.2M. The LANL-developed methodology and its application is the cornerstone of the biological

risk assessment that was delivered to the President in January 2005. The success in this project has also led to \$3.2M of funding in FY05 for an applied research program to develop a rapid risk assessment capability for the Nation, also led by T Division and drawing heavily on the long standing capabilities in group T-10. In addition, the project is the impetus for the basis of a FY06 Congressional Initiative to develop a Center for Theoretical and Computational Pathomics (ranked number one in the Laboratory's DoD initiatives). Taken together, these projects and initiatives define a vision and path forward for the biosciences at the Laboratory, as well as addressing critical national needs in homeland security.

The second project (EpiCast) included in the PM 4.4 deliverables is the establishment of new epidemiological modeling capability that can assimilate data from the public health monitoring systems and forecast the future of an epidemic. It addresses two unmet needs of the Nation's biodefense: (1) providing a tool to decision makers to weigh mitigation strategies during a crisis, and (2) understanding the coupling between local events and national consequences. The project originated in a DOE program for the support of Homeland Security (CBNP) and was transferred to DHS Science and Technology when it stood up. The deliverable for the measure is:

Develop and apply an advanced simulation capability to aid in planning and understanding response to contagious disease outbreaks, in support of the DHS Biological Countermeasures portfolio.

While the main deliverables are to be provided at the end of FY05, DHS considered this project to be of such key importance that the budget for FY05 was doubled to \$1M (no other project in the \$60M portfolio had such a large increase). Because of the immediate need of the tools developed in this project, its timeline was restructured to provide resources earlier. Critical in this development was the use of a simulation resource that was developed for the NW programs for simulating molecular dynamics (SPaSM), but which proved to be so remarkably flexible that it was quickly adapted to modeling epidemics resolved at an individual level. The resulting capability was demonstrated to be capable of modeling the entire world's population (billions of people), where the comparable state of the art in the world is attempting to model regions of the U.S. (millions). EpiCast will also be the core epidemiological capability for a highvisibility incident awareness capability that is being developed for cities around the US to support the integration of the BioWatch environmental surveillance system with the local public health and emergency resources.

PM 4.5. Apply advanced science and technology to meet immediate and long-term US defense community needs.

Advances made by Division staff in the areas of quantum encryption and quantum key distribution continue to receive support (from NSA, DARPA, LDRD) and are excellent examples of advanced science and technology being applied to general defense and intelligence community needs. While our contributions in this general arena are often small in scale, they are generally of very high impact.

PM 4.6. Maintain and deploy, as required, nuclear emergency response teams for CONUS and OCONUS response to radiological and nuclear threats.

Members of the Division continue their relationship with the Emergency Response community.

Performance Objective #5: Enhance and nurture a strong science, engineering, and technology base in support of national security strategic objectives.

The nature of the programs T Division is involved with varies from the core program that initiated the Laboratory (the nuclear weapons program), to medium-sized, multidivisional programs (most recently in Threat Reduction and Homeland Security) to small, innovative programs at the cutting edge of science. A major role of the Division has been and remains that of innovator and incubator for future technical directions of the Laboratory. Frequently these projects reach a level of development that attracts significant program funding and consequently have even led to the establishment of new Laboratory divisions. For example, X (Applied Physics), CCN (Computing, Communications and Networking), CCS (Computer and Computational Sciences), and D (Decision Applications) divisions had their origins in T Division.

PM 5.1. Nurture and maintain the Laboratory science and engineering excellence in disciplines and capabilities needed to support our national security missions and emerging national needs.

There are a number of statistical measures that demonstrate the Division's efforts in nurturing, maintaining, and supporting excellence in science capabilities and technical staff.

Research papers and reports. Each year, T Division staff produce approximately 30% of all the peer-reviewed publications at the Laboratory. T Division makes a diligent effort to record all publications for each calendar year. Division staff members contributed to almost 700 publications in 2004; Appendix A (see page 40) contains a list of these publications. Because each group reports its own publications and some publications have authors from two or more groups, we may accumulate some duplicate records although an effort has been made to remove duplicate entries. These approximately 700 publications represent an average of almost three peer-reviewed publications per Technical Staff Member and Postdoctoral Associates within the Division. From this list the tremendous breadth and quantity of the published research from Division staff is readily apparent, as is the very broad range of journals in which they publish. Clearly, biologists will read and publish in different journals than do atomic physicists or computer scientists. Indeed, one of the strengths of the Division is the close associations and collaborations among scientists from many different disciplines. Thus, statistics on which journal is most commonly chosen for publication is substantially different for T Division than for an organization that has only a limited set of programs, and will also vary from year to year as research interests evolve. Journals of the American Physical Society are the most common, as is the *Physical Review Letters* journal (approximately 220 articles appeared in one of the five volumes of the *Physical Review*).

GROUP	NUMBER OF PUBLICATIONS
T-DO	43
T-1	26
T-3	8
T-4	52
T-6	24
T-7	65
T-8	40
T-10	83
T-11	94
T-12	109
T-13	67
T-14	15
T-15	24
T-16	34
CNLS	16

A sense of the disciplines in which there is the greatest activity can be gained by compiling a list of the number of publications in each group as shown in the following table. This is, of course, a broad generalization because some staff work in more than one discipline, disciplines extend over more than one group, and some groups work on activities in which it is difficult to publish in the open literature.

Not all the unclassified research output of the Division appears in peer-reviewed journals. Appendix B (see page 74) contains a list of all publications, reports, and preprints for which a Laboratory information release number (LAUR) was requested during 2004. Even this list does not completely represent the sum of the Division's publication and presentation output. Approximately 36% of the Division's budget is derived from the Nuclear Weapons Program, which supports some work that cannot be published in the open literature or is in support of the Division's three major database efforts. Much of that work will appear in the form of the classified or unclassified databases, classified reports, or classified papers. Division staff members wrote a total of 22 classified reports and papers in 2004, which are listed in Appendix C (see page 128). In addition, some of our work for industrial sponsors may be proprietary and is also not normally publishable in the open literature.

<u>Presentations and invited talks.</u> The distinction between invited talks and other presentations is often difficult to ascertain. At some meetings the distinction is clear and relevant while not in others. Because such efforts

would be subject to considerable error, we have not attempted to track this distinction in our database. The list of presentations at professional meetings and conferences is provided in Appendix D (see page 130), reflecting the major international involvement of the Division's staff. In addition to presentations at professional meetings, staff also frequently make presentations to UC and government officials and program sponsors throughout the year.

Awards, honors, and elections. Members of the Division who received awards and honors during 2004 are listed in Appendix E on page 170. Elections to national science and engineering societies are also included. Of special note for 2004 is Bette Korber's (T-10) DOE Ernest Orlando Lawrence Award, which she received in the Life Sciences category, and Wojciech Zurek's (T-DO) Phi Beta Kappa Visiting Scholar award.

In 2004, three new Laboratory Fellows were appointed from within T Division: Alan Bishop (Division Leader), Byron Goldstein (T-10), and Joseph Carlson (T-16). The quality of the senior Division staff is reflected in the fact that a much larger fraction of our staff are Laboratory Fellows relative to the number in other divisions. In 2004, T Division had

5 Senior Fellows and 30 Fellows (including retirees). Following is a list of members and associates of the Division that are Fellows or Senior Fellows of the Laboratory.

SENIOR FELLOWS				
Colgate, Stirling A., T-6	Perelson, Alan S., T-10	Younger, Stephen M., T-DO		
Frauenfelder, Hans, T-10	West, Geoffrey B., T-8			
	FELLOWS			
Baker, George A., T-11	Friar, James L., T-16	Pack, Russell T., T-12		
Bishop, Alan R., T-DO	Goldstein, Byron, T-10	Smith, Darryl L., T-11		
Boulaevskii, Lev, T-11	Ginocchio, Joseph, T-16	Solem, Johndale, T-DO		
Brackbill, Jeremiah U., T-3	Harlow, Francis H., T-3	Strottman, Daniel, T-DO		
Carlson, Joseph, T-16	Hay, P. Jeffrey, T-12	Swartz, Blair K., T-7		
Collins, Lee, T-4	Hills, Jack, T-6	Voter, Arthur F., T-12		
Cowan, Robert D., T-4	Kober, Bette, T-10	Wallace, Duane C., T-1		
Cox, Arthur N., T-6	Louck, James D., T-7	Wendroff, Burton, T-7		
Dukowicz, John K., T-3	Milonni, Peter, T-DO	Young, Phillip G., T-16		
Ecke, Robert E., CNLS	Nieto, Michael J., T-8	Zurek, Wojciech, T-DO		

Memberships in professional organizations. Numerous staff members in the Theoretical Division are members of one or more professional organizations, with 34 of them elected to the rank of Fellow within these organizations. A list of organizations and the Division members in those organizations are listed in Appendix F on page 174. A summary of these memberships by organization is shown below.

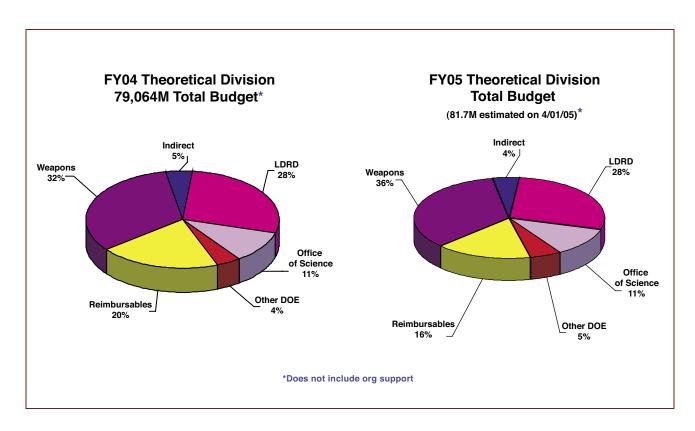
Organization/Society	T Division Members	T Division Fellows
AIDS Vaccine Research	1	
American Academy of Arts and Sciences	1	
American Association for the Advancement of Science	13	1
American Association for the Study of Liver Diseases	1	
American Association of Immunologists	3	
American Association of Physics Teachers	1	
American Astronomical Society	9	
American Chemical Society	23	
American Geophysical Union	6	
American Institute of Aeronautics and Astronautics	1	
American Institute of Chemical Engineers	1	
American Institute of Physics	1	1
American Mathematical Association	1	
American Mathematical Society	11	
American Meteorological Society	1	
American Nuclear Society	2	
American Philosophical Society	1	
American Physical Society	93	28
American Society for Metals	1	
American Society for Microbiology	1	

Organization/Society	T Division Members	T Division Fellows
American Society of Mechanical Engineers	4	
Association for Women in Mathematics	1	
Astronomical Society of the Pacific	1	
Atomic Energy Society of Japan	1	
Biophysical Society	7	1
California Alumni Association	1	
Canadian Applied Mathematics Society	1	
Division of Plasma Physics	1	
DYMAT Association	1	
European Center for Theoretical Studies in Nuclear Physics and Related Areas	1	
German Physical Society	2	
Great Lakes Bioinformatics Consortium	1	
Industry-University Cooperative Research Program	1	
Institute of Electrical and Electronics Engineers	2	
Institute of Mathematical Statistics	1	
Institute of Physics (UK)	2	1
International Association of Computational Mechanics	2	
International Association of Hydrological Sciences	1	
International Astronomical Union	3	
International Society for Genetic and Evolutionary Computation	1	
Israel Association for the Study of the Liver	1	
Israeli Society for Theoretical and Math Biology	1	
Leopoldina Academy	1	
London Mathematical Society	1	
Materials Research Society	6	
Mathematical Association of America	2	
National Academy of Sciences	1	
National Institute of Allergy and Infectious Diseases	1	
Optical Society of America	1	1
Physical Society of Japan	1	
Protein Society	1	
Royal Astronomical Society of London	1	
Royal Society of Chemistry	1	
Royal Swedish Academy-Foreign Member	1	
Santa Fe Institute	2	
Sigma Xi Scientific Research Society	7	1
Society for Advancement of Chicanos and Native Americans in Science	5	
Society for Industrial and Applied Mathematics	28	
Society for Mathematical Biology	4	
Southwestern Quantum Information Technology (SQuInT)	1	
Swiss Physical Society	1	

Organization/Society	T Division Members	T Division Fellows
The Minerals, Metals & Material Society	2	
Topical Group on Shock Compression of Condensed Matter	1	
Tsunami Society	1	
UC Engineering Alum. Society	1	
Union of Concerned Scientists	1	
U.S. Association of Computational Mechanics	3	

PM 5.2. Develop and implement an integrated and balanced strategy for investing LDRD, programmatic and institutional resources to ensure the long-term vitality of the Laboratory science, engineering, and technology base in support of national security missions and emerging national needs.

T Division pursues a balanced research portfolio that includes LDRD, Weapons Program, Threat Reduction programs, and other sponsors and agencies in the DOE, NIH, NSA, NASA, and industry, among others. This portfolio has allowed the Division to interact strongly with both the academic community in areas of basic research, with designers in the weapons programs, and with customers in threat reduction and homeland security. This broad spectrum of research has provided a conduit that has facilitated transfer of new ideas and techniques from basic research into the applied programs throughout the Laboratory.



Researchers in T Division have successfully competed to acquire significant LDRD funding, which has allowed the Division to support and nurture a large number of innovative research directions. Many of these initiatives may later expand the capability for current programmatic efforts. These LDRD projects have also led to numerous publications, which are included in Appendix A (page 40). LDRD support has been crucial in attracting and maintaining gifted and highly motivated researchers within the Division. The following table shows the "new-start" FY05 LDRD projects with T Division involvement. (These contribute to approximately one-third of the total Division LDRD portfolio.)

Title	PI	PI Group	T Division Participants
Rational Vaccine Design: Theory and experimental validation	Bette Korber	T-10	T-8: T. Bhattacharya; T-10: A. Perelson, R. Ribeiro, B. Korber, G. Gnanakaran, B. McMahon, C. Kuiken; T-13: A. Lapedes
Physical Modeling of Biomolecules and Ribonucleo-protein Complexes of Importance to Pathogenicity	Benjamin McMahon	T-10	T-10: M. Labute, K. Sanbonmatsu, G. Gnanakaran, B. McMahon; T-12: K. Nemeth
Nanoscale Fluctuations in Multifunctional Materials	Alexander Balatsky	T-11	T-11: K. Rasmussen, J. X. Zhu, S. Trugman, D. Smith; T-10: K. Sanbonmatsu
Atomistic Studies of Fast Chemical Processes in Nanostructured Metastable Composites	Alejandro Strachan	T-14	T-14: S. Zhao
New Americium Delta-A Metric for Primary Certification (U)	Mark Chadwick	T-16	T-16: T. Kawano, P. Talou, P. Möller, E. Lynn
A System-scale Theory for Fast Magnetic Reconnection	Dana Knoll	T-3	T-15: L. Chacon
Coming Out of the Cosmic Dark Ages - The First Stars in the Universe	Alexander Heger	T-6	T-6: C. Fryer, M. Warren, S. Colgate, G. Jungman, F. Timmes, T. Luu, B. O'Shea, D. Whalen; T-7: S. Li; T-8: A. Friedland; T-16: J. Carlson, S. Reddy, P. Möller
Antineutrino Monitoring of Reactors	Anna Hayes-Sterbenz	T-6	T-6: G. Jungman, J. Hills; T-8: M. Nieto; T-16: B. Wilson, S. Cowell, A. Steiner
Cross Sections for the Isomer of 235U	Anna Hayes-Sterbenz	T-6	T-6: G. Jungman, J. Hills; T-16: J. Friar
Taming and Accelerating Particle-In-Cell	Salman Habib	T-8	
Measuring Neutrino Properties with Oscillation Experiments	Tanmoy Bhattacharya	T-8	T-8: A. Friedland
Cold Atom Quantum Simulators	Juan Paz	T-DO	T-4: D. James, E. Timmermans; T-11: G. Ortiz, J. Gubernatis
Lagrangian Measurements of Fluid Mixing	Robert Ecke	CNLS	T-13: M. Chertkov, D. Sharp, B. Plohr; T-11: P. Lomdahl; T-12: B. Holian; T-14: K. Kadau, J. Barber
Nonlinear Behavior in Complex Systems	Robert Ecke	CNLS	Postdocs
Cooperative Phenomena in Soft Matter	Robert Ecke	CNLS	Postdocs
Resolving the Aerosol-Climate-Water Puzzle: Predictive Science for Global Stability and Security	Manvendra Dubey	EES-6	T-3: P. Jones; T-7: D. Moulton
Pu-H Interactions: Studies of Plutonium Hydride Phenomena (U)	David Moore	NMT- 16	T-1: SP. Chen; T-12: J. Hay, R. Martin
Protocell Assembly	Steen Rasmussen	EES-6	T-6: S. Colgate; T-7: Y. Jiang; CNLS: P. Weronski
Material Response During Dynamic Loading at Subpicosecond Time and Nanometer Length Scales	James Glownia	DX-2	T-4: S. Mazevet; T-11: R. Albers
Be-Specific Human Immune Response and Development of CBD	Thomas McCleskey	C-SIC	T-10: S. Gnanakaran; T-12: D. Asthagiri, L. Pratt

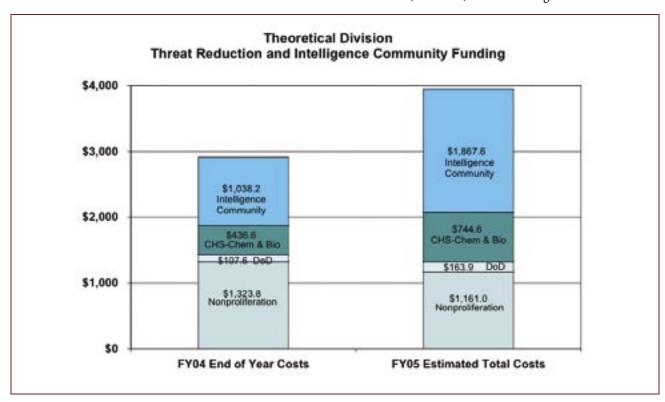
Title	PI	PI Group	T Division Participants
	m		m c o n
Thinking Telescopes: Pursuing a New Paradigm for Discovery in Observational Science	Tom Vestrand	ISR-1	T-6: C. Fryer, M. Warren
Fulde-Ferrell-Larkin-Ovchinnikov Inhomogeneous Superconducting State	Roman Movshovich	MST-10	T-11: L. Boulaevskii
Physics of Astrophysical Jets	Hui Li	X-1	T-6: S. Colgate; T-7: S. Li; T-15: J. Finn, G. Lapenta

Work in the Threat Reduction programs is often classified, but significant recent efforts have been described under Performance Objective #4 (see pages 20-22). The creation of the Laboratory's CHS, and renewed activities with DoD agencies, have allowed the Division to considerably expand the Division's role as described earlier in this document. This involves use of our expertise in computation, modeling, simulation and networks; novel chemistry and materials; biological databases and physics; nuclear and radiological processes; and other areas. The Division also nurtures and maintains an active research effort in energy and environmental science such as modeling ocean currents and climate change.

PM 5.3. Execute non-NNSA sponsored research and development that builds on unique Laboratory expertise and capabilities and enhances the ability to meet current and future national security needs.

The Division's evolving funding portfolio is another demonstration of how successful it has been in the pursuit of non-NNSA-sponsored research and development. The staff have successfully pursued opportunities to work with industry or other agencies with great celerity. New opportunities in Homeland Defense and Threat Reduction have also been vigorously pursued (described above), in addition to the continuously strong Work for Others/Reimbursable (DOE, NIH, NSA, NASA, etc.) portfolio.

T Division has been very responsive to changing national needs with respect to research in nuclear weapons, energy, environmental change, industrial competitiveness, terrorist threats, disease epidemics, and other challenges. The support of these varied research missions has further allowed the Division to attract, motivate, and maintain gifted researchers



with a wide range of research skills. The Division is committed to maintaining and growing its capabilities to respond to new research challenges of national importance and has aggressively pursued sponsorship of research to build upon and enhance its capabilities.

Laboratory's National security goals. The Division contributes in a wide variety of ways to all of the seven Laboratory goals, as evidenced throughout this document. The breadth of research capabilities throughout the Division allows us to respond to questions, problems, and programs that relate directly to one or more of the goals. A good set of examples is the databases that are the responsibility of T Division: equation-of-state, nuclear cross sections, opacities and other photo cross sections, and the AIDS and papilloma virus databases. Other examples involve new projects with the Decision Applications (D) Division in agent-based modeling, with applications including epidemiology and critical infrastructure modeling. There are many more examples to be derived from core theory and modeling problems where analysis and assessment are needed as a phase of problem solving. The new biological threat characterization (DHS) initiatives rely heavily on theory, modeling, and databases from T Division (see PM 4.4 on page 21).

<u>Interactions with industry.</u> Despite the decline of CRADA initiatives nationally, staff throughout the Division remain actively engaged in responding to collaborative opportunities with industry. Division staff have made scientific contributions to US industry, including partnering with Proctor & Gamble, petrochemical firms such as Exxon-Mobil and Dow Chemical, and automobile manufacturing giants such as Ford and Daimler-Chrysler on computer simulation of manufacturing processes and product performance.

Non-Federal Work for Others Agreements: 13 active agreements, 4 executed in 2004.

Agreement No.	Partner	PI and Group	Information
FIA-04-003	St. Jude Children's Research Hospital	Catherine Macken T-10	Executed 5/2004 Scheduled expiration 8/2005
FIA-04-026	The Regents of the University of New Mexico	Alan Perelson T-10	Executed 6/2004 Scheduled expiration 6/2005
FIA-04-036	The General Hospital Corporation (<i>dba</i> Massachusetts General Hospital)	Bette Korber T-10	Executed 9/2004 Scheduled expiration 11/2009
FIA-04-047	Acta, Inc.	B. VanderHeyden T-3	Executed 12/2004 Scheduled expiration 12/2006

Nondisclosure Agreements: 2 active agreements, 1 executed in 2004.

No.	Partner	PI and Group	Information
4808	The University of Hong Kong	Alan Perelson T-10	Executed 2004 Scheduled expiration 6/2006

Patent Applications and Issued Patents: 1 application filed and 1 issued in 2004.

DOE S-Number	Title	Inventors and Group	Application Type Filing Date
100635	Software and Procedures for Creating Mathematical/ Computational Models of Cellular Signaling	William Hlavacek (T-10) James Faeder (T-10) Mikhail Blinov (T-10)	ORD 19 Aug 2004
DOE S-Number	Title	Inventors	Issue Date
94780	Methods and Optical Fibers that Decrease Pulse Degradation Resulting from Random Chromatic Dispersion	Ildar Gabitov (T-7) Michael Chertkov (T-13)	2 March 2004

Invention Disclosure: 1 invention disclosure in 2004.

LAD#	Title	Inventor	Status
2003112	Polyvalent Immunogen	Bette Korber (T-10)	Pending

Copyright Assertions: 1 copyright assertion submitted in 2004.

DOE-C-No.	Code Name	Author
C-04,012	Mesh Toolkit (MSTK), Version 1.2	Rao V. Garimella (T-7)

CRADAs: 2 continuing CRADAs, which are described below.

Advanced Multifield Simulation Development (Proctor & Gamble and Sandia National Laboratories; Principal Investigator Bryan "Bucky" Kashiwa, T-3; expected completion, August 2005)

The collaborative research performed under this CRADA will develop new approaches to addressing issues in manufacturing, materials development and use, biosciences and computer-based simulation of physical processes. The T Division work, performed under the aegis of the Laboratory-wide CRADA, is to scope the use of certain cutting-edge developments in multi-field flow theory on manufacturing problems of interest to Proctor & Gamble. Of particular importance are models and methods for examining the dynamics of solid materials influenced by the flow of a turbulent gas stream, a closely coupled fluid-structure interaction. This ongoing work is valued by Proctor & Gamble for reducing the cost of engineering new manufacturing processes. At the same time the work provides positive feedback to the Laboratory by testing new theories and simulation methods in flow regimes relevant to our mission.

Manufacturing of Model-Driven Nanostructured Materials (Metallicum, LLC; Principal Investigator Irene J. Beyerlein, T-3; expected completion, October 2006)

Under a DOE project, Initiatives for Proliferation Prevention, Los Alamos (T-3) and scientists in the former Soviet Union are working to develop predictive models for advancing understanding and optimal design of severe plastic deformation (SPD) technologies. The SPD process used by Metallicum, LLC, called Equal Channel Angular Processing (ECAP), can potentially produce nanostructured metals with the extraordinary property of simultaneous ultrahigh strength and high ductility as well as superplastic forming behavior. Together Metallicum, LLC, and T-3 are managing and technically guiding Russian scientists in model development. The models will enhance US competitiveness via lower experimental costs and more optimal and efficient manufacturing processes. Moreover, they will help to transfer SPD processes to the market by providing reliability and efficiency. Currently, Metallicum, LLC, is the only company who intends to sell metals made by these processes.

Support of energy resources. Currently, the Division has one automotive effort supported by the DOE Office of Energy Efficiency and Renewable Energy (EE). The effort is improving the engine simulation software, KIVA, by increasing the types of grids KIVA can compute with and reducing computer simulation times by parallelizing the code.

Several Division staff are working in support of the Global Nuclear Futures Initiative, the goal of which is the transmutation of high-level waste to shorter-lived, low-level waste. Under this program, spent nuclear fuel from commercial power plants would be chemically separated and the actinides sent as feed stock to advanced nuclear systems, either reactor-based or accelerator-driven, to be fissioned. Such a scheme would greatly reduce the amount of high-level waste that would normally be bound for an underground repository, as is the current practice in the US. The Global Nuclear Futures Initiative is being spearheaded by the ADSR and has successfully received the backing of the Laboratory. A more detailed program plan is currently being developed, partially in conjunction with other laboratories including the Idaho National Engineering and Environmental Laboratory, and LANL is working with congressional delegations to obtain support for it as a national policy direction. From a technology perspective, this is a very broad initiative and draws on many strengths in the Division including the nuclear physics associated for developing new nuclear data evaluations for the design of new reactors and to support the transmutation processes, nuclear fuel design, materials issues associated with behavior in hostile environments, and novel algorithms for the solution of coupled nonlinear implied equation systems for the next generation of nuclear reactor safety simulation models.

Support of environmental quality. Division management are members of the Laboratory's Energy and Environmental Council. As mentioned above, Division staff are involved with the automotive companies to help design a cleaner and more efficient internal combustion engine. A novel method of sequestering CO₂ from the flue gases of coal burning power plants has been extended to include possible removal from the atmosphere. Several Division staff were active participants in the AAA project, which when built will convert long-lived radioactive elements into short-lived products as well as produce electrical power. Other projects are the development and application of numerical methods for multicomponent spray evaporation to be utilized to analyze internal combustion engines.

T Division hosts half the members of the LANL **Climate, Ocean and Sea Ice Modeling (COSIM) project.** Ocean and sea ice models developed by COSIM are used in several of the world's leading global climate models. Predictions from these models are contributing to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, the most important confluence of international climate modeling expertise. COSIM models are also used by Division researchers to study polar processes by participating in the **Arctic Ocean Model Intercomparison Project,** which involves over a dozen international modeling groups. Most climate models predict maximum warming in the polar regions, and there is much evidence that polar warming has already begun. As sea ice thins and retreats, changes in the heat and fresh water content of the polar oceans could have a profound influence on the ocean circulation and climate.

Division researchers are also building on their reputation in high-resolution ocean modeling by embarking on the most ambitious coupled **ocean circulation/ecosystem simulation** ever attempted. By combining a realistic ocean circulation with marine ecosystem dynamics (including interactions among plankton, nutrients, and inorganic compounds), we will better understand the earth's carbon cycle and the effects of climate change on the marine ecosystem, which lies at the base of the global food chain.

COSIM researchers continue to advance the state of the art in ice and ocean modeling. A hybrid-coordinate ocean model, HYPOP, is being developed to describe the ocean circulation more accurately. This model combines the best features of z-coordinate models, which are most accurate in the upper ocean, and isopycnal models, which excel in the deep ocean. Work has also begun on modeling the ice sheets that cover Greenland and Antarctica. Ice-sheet melting in a warmer climate could substantially increase global sea level.

Support of other federal agencies. The Theoretical Division continues to have significant interactions with the Department of Defense (DoD), particularly on programs requiring a fundamental understanding of underlying physical process, innovative approaches to fundamental questions, and an appreciation of the needs of DoD and its customers. The National Security Agency (NSA) funds three research projects on quantum computation. One is understanding the fragility of quantum information and developing methods to make it more robust against corruption. Already a better understanding of decoherence, one of the main sources of this fragility, has been reached. Quantum error codes have been developed for noise independent from qubits (the quantum version of bits) and the simplest version has been implemented using Nuclear Magnetic Resonance. A theory of quantum error correction for general noise is being developed. A second project is developing a perturbation theory for scalable quantum computation and modeling and simulations of the processing of information in solid-state quantum computers with many qubits. The goal is to define the range of parameters for which the errors are small, to increase our understanding of the effects of errors and to allow benchmarking future quantum computer devices. The third project supports the ion trap effort in the Laboratory's Physics Division, in particular, the heating of ions due to patch potential and stray field are under investigation. Additional projects are classified. Another group is involved with Defense Advanced Research Projects Agency (DARPA), on single-spin based quantum microscope, and with the NSA, on scalable self-assembled quantum computation.

A team in T-6 has been funded by the **National Aeronautics and Space Administration** (NASA) Applied Information Science Research Program to develop tools to store multiterabyte datasets as cost-effectively and efficiently as possible. This 3-year project, Software Technology to Enable Reliable High-Performance Distributed Disk Arrays, has the goal of building disk arrays out of commodity off-the-shelf hardware to reduce storage cost by a factor of 10. T-16 researchers have also won a 3-year grant from NASA to develop nuclear modeling codes that simulate nuclear reactions from high-energy protons and ions in space environments. These simulation codes use intranuclear cascade theory to model the break-up processes and also include models for break-up of the ion projectiles and decay mechanisms such as spallation and fission.

Since 1986, the Division has received funding from the AIDS Division of the National Institutes of Health (NIH) to provide a sequence database and analysis resource for the international AIDS research community (http://hiv-web. lanl.gov). The database is currently serving thousands of researchers and institutions in over fifty countries and has tens of thousands of users each week. One of the principal services of the database is in the realm of a discipline known as molecular epidemiology, the global tracking of infectious pathogens. Thus, the database and analysis unit is also the World Health Organization's (WHO) database for molecular information pertaining to the AIDS pandemic. Since its inception, T-10 has steadily added more databases to its repertoire. Presently, they curate a database of HIV immunological epitopes, a database of mutations associated with resistance to antiretroviral drugs, and a database of HIV and SIV vaccine trial data. With these databases come ever-growing sets of tools to facilitate data analysis and a collection of review articles by experts in the field, tutorials, etc. For each database, T-10 produces a yearly compendium providing a synopsis of the data. These compendia are provided free of charge to subscribing institutions and scientists worldwide. Based on a summary of the global diversity captured in the database, we are helping in the design of vaccine reagents for HIV. Molecular sequence and immunology databases for infectious pathogens are a first line of defense in this modern war against plagues. As an extension of the HIV databases, the NIH has funded a new database project in Hepatitis C virus. The WHO estimates some 170 million people carry HCV and there is currently no vaccine against Hepatitis C or HIV.

PM 5.4. Foster active participation in the broad scientific and technical community, leveraging unique Laboratory expertise and capabilities; develop strategic collaborations with other national laboratories, industry, and academia.

All technical staff members in the Division are involved in collaborations with the scientific community (universities, industry, and other national laboratories) throughout the world (see Appendix G on page 184). In addition, several members of the Division also serve as officers in the societies of which they are members. Division staff also engage in personnel exchanges with industry and other federal laboratories and agencies as temporary staff on "Change of Station" assignments as program managers at NSF, NIH, and the NNSA.

T Division staff are also involved in a great number of external interdisciplinary programs, for example, the University of California Cooperative Agreement on Research and Education (CARE) program, which is designed to identify and fund opportunities for promising students and faculty to participate in new and innovative research, enhance collaborations with universities in areas of strategic importance, and provide a research environment to encourage students to pursue technical careers. Division staff are closely involved in the Santa Fe Institute's (SFI) multidisciplinary programs and have played a seminal role in the Institute's foundation, along with continuing activity through collaborations and organization and participation in conferences. In 2004, a SFI/LANL Memorandum of Understanding was executed, which was based on negotiations led by T Division. The newly founded NSF Center at the University of New Mexico (UNM) for the Consortium of the Americas for Interdisciplinary Research was the result of a strong partnership between UNM and Los Alamos where T Division played the major role. Division staff serve on the Governance Board of the new UC/LANL Memoranda of Understanding with UCSD, UCSB, UCD, UCSC, and UCR campuses.

The Theoretical Division is a partner in the National Science Foundation Nanoscale Science and Engineering Center (NSEC) for Directed Assembly of Nanostructures at Rensselaer Polytechnic Institute and the University of Illinois at Urbana-Champaign, founded in September 2001. The mission of the center is to integrate research, education, and technology dissemination, and serve as a national resource for fundamental knowledge and applications in the directed assembly of nanostructures. The center research involves two major areas of emphasis: nanoparticle gels and polymer nanocomposites and nanostructured biomolecule composite architectures. Several staff members in the Division participate in the partnership and Antonio Redondo (T-10) is a member of the Executive Committee of the Center.

The Division hosts half of the members of the LANL Climate, Ocean and Sea Ice Modeling (COSIM) project. Ocean and sea ice models developed by COSIM are used in several of the world's leading global climate models. Predictions from these models are contributing to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, the most important confluence of international climate modeling expertise.

Important new projects started in T Division by the DOE Office of Science in FY05 include (1) a theory, modeling, simulation element of CINT (with Sandia National Laboratories [SNL]); (2) organic electronic materials; and (3)

solid-state lighting (with SNL). New projects funded by NIH include a joint project with the **Harvard Medical School** on transcription in DNA. Division collaborations with **industry** are described in PM 5.3 on page 28.

Examples abound of the more **informal involvements** in interdisciplinary programs. This includes: (1) sponsorship of conferences and workshops to bring together experts from several disciplines around the world; (2) fostering new collaborations in materials science involving materials modeling with accurate chemistry now deployed in the ASC and other programs; and (3) frequent interchange of information and ideas between Division staff and the rest of the Laboratory (including internal sabbaticals with X Division and several joint appointments).

<u>Editorial boards</u>. At least 37 members of T Division serve on editorial boards of over 50 different professional journals in a variety of capacities. A detailed list is given in Appendix H on page 210.

<u>Referees on journals and other publications.</u> Division staff also serve the larger scientific community by serving as referees on over 80 different journals and other publications. Over 50 individual staff members serving in this capacity are shown in Appendix I on page 214.

<u>Professorships, committees and boards.</u> T Division staff continue to remain active in the external research community by serving on a wide variety of technical committees and advisory boards. Many of the Division's staff members also hold adjunct professorships with academic institutions. These relationships not only foster scientific exchanges and collaborations, but also serve as effective recruiting mechanisms. A list is provided in Appendix J (see page 220).

<u>Conferences</u>. The Division continues to host and/or organize a broad variety of **conferences and workshops** designed to foster active participation by a wide range of collaborators and potential collaborators in academia, other research laboratories, and industry. These number at least 20 per year; in August 2004, for example, the Division hosted the 12th International Conference on Recent Progress in Many-Body Theories in Santa Fe. In addition, the Division is responsible for organizing several annual educational programs for students in mathematics, physics, and biology. These education programs are described in Performance Objective #10 (pages 36–38).

T Division, in collaboration with the Laboratory's Physics Division, hosts the **P/T Colloquium** series. This series has been ongoing for over 10 years and has brought a wide variety of distinguished speakers to Los Alamos. The talks are open to the entire Laboratory community and are always well attended. In 2004, T Division hosted about half the speakers out of the total 33 talks given during the year.

Another regular series hosted and organized by the Division is the **Quantum Lunch**, which features speakers from different organizations and academia with an interest in fostering continued collaborations and research and development in the quantum information science and technology field. These informal presentations and interactions occur approximately three times per month. In 2004, 32 talks were hosted. This lunchtime series is part of the Laboratory's Quantum Institute, which was formally organized in 2002 with the mission of providing advocacy, information, coordination, and organizational support for quantum information science and technology programs and researchers at Los Alamos. The Los Alamos Quantum Institute embodies the single largest multidisciplinary collection of quantum information science and technology researchers in the world. T Division is one of seven Laboratory divisions currently participating in the Institute.

A listing of conferences and workshops, P/T Colloquium talks, and Quantum Lunch talks for 2004 is given in Appendix K on page 226.

Code/software products. Several of the Division's projects involve the design of software packages or computer algorithms. In some instances these are packaged and made available for the general research community. Many of T Division's products are used in institutions around the world and are the benchmarks against which other codes or methods are compared. Two examples of such software packages are CAVEAT and NJOY. CAVEAT is a 3-D hydro program used in many applications, NJOY is a data-processing package for nuclear reaction data. Other examples include OpenSesame, a suite of equation-of-state tools, and the accompanying Sesame Library, a compendium of equation-of-state tables used by government, academic, and industrial institutions. LAGriT (Los Alamos Grid Toolbox) is a set of tools for creating and tracking unstructured grids in multimaterial applications, used by many academic institutions.

Performance Objective #6: Optimize current and evolving mission performance by providing effective and efficient facilities and infrastructure.

Although T Division certainly relies on efficient facilities and infrastructure to carry out its work, the Division does not have significant involvement in ensuring this Performance Objective is met.

Performance Objective #7: Utilize UC strengths to recruit, retain, and develop the workforce.

PM 7.1. Recruit and retain a skilled and diverse workforce that meets the Laboratory' long-range core and critical skills requirements by implementing a human resource strategy that leverages student programs and UC relationships.

The Division aggressively participates in the Laboratory university recruitment program by advertising in professional journals and fully utilizing its extensive network of professional colleagues inside and outside the Laboratory. The principal mechanism for hiring technical staff is through a deliberate use of the Graduate Research Assistant and Postdoctoral Associate programs as a systematic pipeline. This has been an extremely useful and successful recruiting tool as the quality of the current staff demonstrates. In 2004, the Division converted eight Limited-term Technical Staff Members (LTSM) to full-time, regular (TSM) employee status and seven Postdoctoral Associates to either LTSM or TSM status. A small number of technical staff (approximately 20%) are recruited directly as LTSMs or regular TSMs. In addition, T Division has historically been extremely successful in recruiting post-docs through the Director's Funded Postdoctoral Fellow Program, as well as garnering a large number of Distinguished Postdoctoral Appointments. All current post-docs and appointment types are shown in Appendix L on page 234. The importance of mentoring and a recruitment pipeline to sustain critical capabilities are considered strategically essential by T Division.

PM 7.2. Implement leadership and management development programs that achieve workforce and diversity objectives.

The Laboratory has recently initiated several leadership and management development programs and T Division has been actively participating as they evolve. In 2004, two Division members (Brian VanderHayden, T-3, and Audrey Archuleta, T-DO) were active in the new (2003) Director's Development Program, which is aimed at addressing the specific need to better prepare individuals to effectively transition to progressively higher levels of management. T-6 Group Leader, Frank Timmes, was elected to serve as the 2004 Vice-chair of the Group Leader Action Council, which reviews a wide variety of topics and proposed policy changes that affect line management at the Laboratory. He will become chair in 2005. Several Division members have attended the Laboratory's Leadership Institute and Management Institute training and development series.

During 2004, several changes in Division group management occurred due to promotions to serve in broader Laboratory capacities (including Deputy Chief Science Officer of the Laboratory and an ASC Program Manager), or other careerchoice changes. The next generation of group line managers has been easily recruited from within the Division, as they are regularly nurtured through Deputy Group Leader positions, acting positions, or other leadership opportunities (e.g., leading Division thrusts). Where necessary, the Division also recruits aggressively outside the Division or Laboratory to ensure we meet our workforce and diversity objectives.

PM 7.3. Establish and implement a weapons point of contact development program.

The Division has been assuming an ever-greater role in both the execution of the nuclear weapons program plan, but also in its planning and leadership. Over the past five years or so, the Division has gone from no leadership role in the NW program to the current state where a program manager is a T Division alumni and at least six staff members are serving as project leaders or principal investigators. In addition, the Division Office serves as part of an advisory body to the ASC program, the "G4." As a result, we now have a cadre of staff experienced in program and project management, and a development path for future leaders for NW program management.

Performance Objective #8: Maintain safe, secure, environmentally sound, effective, and efficient operations in support of mission objectives.

PM 8.1. Achieve continuous improvement in ISM System performance.

T Division line managers are cognizant of and active participants in the Integrated Safety Management System to ensure performance and appropriate involvement of workers. Line managers make monthly use of the Management Walkaround System (MWA) and engage employees by selecting one or two to accompany them on walkarounds and by discussing safety and security topics with workers they encounter during regular visits. Division MWA compliance rates averaged 138% over the four quarters in 2004, which is well above the Laboratory average. The Division also makes use of the Laboratory's Nested Safety and Security Meeting process appropriate to the activities of the Division and allows a forum for employees to raise issues and make suggestions for safety improvements. Because the work performed in the Division is primarily "office work" (as opposed to experimental work in a laboratory or other facility), it is important to use a tailored approach to Laboratory initiatives to ensure direct relevance to employees and keep them effectively engaged at the appropriate levels.

PM 8.3. *Maintain an environmental management program consistent with the DOE-approved baseline, funding levels, policy, and negotiated regulatory requirements.*

The Laboratory began rolling out its Environmental Management System (EMS) in November 2004. Current activities include completing an all-employee training requirement, communicating the nature of the program to employees, and identifying the areas where each Laboratory organization's activities impact the environment. The Division is an active participant in this evolving program, with a similar approach to the ISM System. The nature and environmental impacts of the Division's activities will drive the tailored approach to the EMS to best serve the intent of the program and remain relevant to the Division.

PM 8.4. Achieve continuous improvement in security performance through ISSM and risk management principles.

T Division line managers are cognizant of and active participants in the Integrated Safeguards and Security Management (ISSM) system to ensure performance and appropriate involvement of workers. Approximately 20% of the Division's activities are classified, or are conducted in secure areas. During the July 2004 Laboratory standdown, security across the Division was a major focus of our Management Self-Assessment. ISSM-related activities included:

- Antonio Redondo (T-10) and Paul Dotson (T-DO), both Authorized Derivative Classifiers, set up a process to handle e-mail securely. The process, which was implemented in consultation with CCS, the Materials Science and Technology (MST) and X divisions, was designed to address potential security risks associated with e-mail originating in the Division while still permitting the Division members to carry out ordinary tasks requiring communication via e-mail. Redondo and Dotson created a presentation containing general as well as group-specific information about potential security risks, including written guidelines for staff. The materials were then used in individual training presentations throughout the month of August 2004 to all groups in the Division. Although a direct correlation is difficult to establish, there has since been a marked decrease in related security issues in this area. The Laboratory has since adopted this basic approach.
- Created a team of "classified workers" to evaluate and develop a list of best-practices garnered from other Divisions, which were implemented in the classified computing facilities in the Division.
- The Division contributed significantly in the performance measure to effectively manage accountable Classified Removable Electronic Media (CREM). All three required-CREM audits in 2004 were 100% compliant throughout the Division. The Division also undertook a major effort in 2004 to reduce its CREM inventory from 108 pieces to 33 by May 18, 2004. By February 2, 2005, we successfully completed the transfer of all accountable CREM to the Decision Applications Division CREM Media Library. The Division no longer has accountable CREM residing in T Division space.
- In collaboration with the Laboratory's Office of Internal Security (ISEC), the Division initiated and established a policy governing the Division requirements for all foreign national employee and visitors and hosts thereof. The policy allows the continued involvement of these essential and highly valued Division resources while still ensuring the ability to detect, deter, and mitigate threats of foreign intelligence collection and espionage at the Laboratory.

Performance Objective #9: Improve or maintain effective business processes and systems that safeguard public assets and support mission objectives.

Although not responsible for establishing the Laboratory business processes and systems, the Division plays an important institutional role by effectively utilizing, implementing, and providing process improvement feedback on Laboratory tools and processes. During the Individual Performance Objective phase of the annual Performance Management system, a conscious effort was made to include performance metrics in this area tailored for each line manager throughout the Division. Several Division line managers and the administrative support have enrolled in or taken courses to improve their understanding of the recent changes and requirements in effective business stewardship, and have identified new tools to assist with financial and procurement management. Division employees will continue to work within the Laboratory systems and will also provide suggestions for improvements that help meet the goal of ensuring the safeguarding of public assets while still enabling the support of mission objectives. The Division is also committed to contributing to and supporting the currently evolving components (as applicable to T Division) of the Laboratory's Operational Efficiency Project and the Enterprise Project. For all Division-specific Corrective Action Plans resulting from Management Self-Assessments, we utilize the Laboratory's integrated monitoring program, I-Track, to track and report findings, recommendations, and improvement actions.

Performance Objective #10: Sustain and/or implement effective community initiatives.

The Theoretical Division has traditionally played a strong role in furthering the education of early-career scientists and researchers. During 2004, the Division employed 76 post-docs, 34 GRAs and 10 undergraduate students (in addition to hosting and educating many more through the Division's summer schools and programs described below). Most of our GRAs are at the Laboratory working on their thesis and are formally mentored by Division staff. A list of the current post-docs is given in Appendix L (page 234) and GRAs is given in Appendix M (page 238). It is evident that T Division staff contribute significantly to nurturing a very large number of graduate students and post-docs in broad scientific areas of science throughout the year. Additionally, large numbers of students and post-docs participated in the numerous conferences hosted by T Division (see Appendix K, page 226).

Educational Initiatives. The Division hosted and organized several major educational programs during 2004. Staff across the Division played active roles in organizing strong technical programs, acted as mentors for the students, and, together with external researchers from academia and other national laboratories, presented a wide variety of materials in their respective fields to a broad range of students.

The Los Alamos Summer School's objectives are attracting top-level talent into research careers in the physical and computational sciences. The program focuses on upper-level undergraduate students and meets these objectives through a concentrated format of research and seminars. We attempt to convey a sense of the excitement and importance of the scientific research in general and that are currently conducted at the Laboratory, including our contributions to national and international security through the science-based stockpile stewardship program. The program extends for ten weeks and consists of a mentored research project and a seminar series. The project introduces the student to the basic mechanics of scientific research, while the seminar series consists of a set of lectures by staff and visiting scientists that focus on topical research in various fields of physics. In 2004, 16 students participated in the program, representing 15 different institutions. The 20 mentors came from 13 different Laboratory groups, with 34 lecturers coming from 16 Laboratory groups and from the universities of New Mexico, Illinois, Rochester, and Nevada. The program is a jointly operated educational initiative between the University of New Mexico and the Laboratory. (Contacts: Daniel James, T-4, dfvj@lanl.gov, and Lee Collins, T-4, lac@lanl.gov)

The Mathematical and Theoretical Biology Institute (MTBI) is a joint LANL-Arizona State University intensive summer research experience for students. The program has a strong focus on providing a research experience for minority students and the program is based on mentorship with nationally recognized Chicano, Latino, and Native American role models. The Summer 2004 (June 19-August 14) program hosted 23 undergraduates, 20 graduate students, and 21 university faculty visitors, and was held at the Los Alamos High School. These students represented 29 different academic institutions, with faculty visitors coming from 9 different institutions. The MTBI summer program includes 4 weeks of collaborative learning in dynamical systems, modeling and computational methods, followed by 4 weeks of intensive research during which MTBI students work in teams under the supervision of faculty and experienced graduate students on projects of their own choosing. Upon completion of the research experience, students prepare poster and oral presentations of their work as well as submit technical reports to deliver to the scientific community. (Contact: Mac Hyman, T-7, jh@lanl.gov)

Since 1999, staff in T-8 and T-6 have been organizing an annual **Cosmology Summer Workshop** at St. John's College in Santa Fe. This continuing series of workshops is co-organized with the Theoretical Astrophysics Group at Fermilab and the Kavli Institute for Cosmological Physics at the University of Chicago. The topical workshop for 2004 concentrated on recent developments in cosmology, especially those related to current and expected observational advances, including the cosmic microwave background (CMB), large-scale structure, and dark matter and energy/early universe. The first two weeks were devoted largely to structure formation and the CMB, while the last week focused on dark energy. The workshop format is designed to emphasize discussion with formal pedagogical review and related talks as appropriate, reserving the largest fraction of the day for discussion and informal meetings. To encourage this informality and discussion, attendance is usually limited. For the 2004 Workshop, approximately 85 attendees (including 30 students), representing over 35 institutions, attended. (Contact: Salman Habib, T-8, habib@lanl.gov)

Staff in T-8 have been instrumental in starting the **Los Alamos Strategic Studies Program** (LASSP) to look at present and emerging security challenges. This program brings in distinguished speakers to discuss a number of aspects of security ranging from nuclear weapons to environment to energy to water. It has also organized three international highly successful workshops that discussed issues of terrorism and nuclear weapons. The overarching purpose of LASSP is educational—to develop the next generation of broad strategic thinkers. These workshops bring together world leaders in science, social sciences, medicine, policy, security studies, industry, and government to explore and understand the concerns, challenges, and opportunities of today and tomorrow. The focus of the 2004 workshop on terrorism was Regional Issues and Roles of Networks, and in the words of many of the invited speakers, the best such workshop they had attended. (Contact: Rajan Gupta, T-8, rg@lanl.gov)

Started and sponsored by the Laboratory Fellows in September 2001, the **Frontiers in Science Public Lecture Series** offers four free lectures a year in Los Alamos, Santa Fe, Española, and Taos to ensure that Northern New Mexico residents can attend. The intent of the series is to make people aware that the Laboratory performs research in global warming, AIDS, astrophysics, and a number of other important issues facing the world, in addition to nuclear weapons research. Joe Ginocchio, T-16, has been the coordinator of the lecture series since its inception. (For information on past and scheduled presentations, see http://int.lanl.gov/science/fellows/lectures.shtml.)

Individual staff from throughout the Division participated in Laboratory and **other educational forums**, many of them volunteering their time. Some of these activities are described below.

HIV/AIDS awareness program for local schools. Rajan Gupta, T-8 Group Leader, continued to volunteer his time to present and discuss issues regarding addictions and HIV/AIDS prevention at the Los Alamos Middle and High schools as part of their health classes, volunteers his time as a HIV/AIDS pre-test and post-test councilor for the New Mexico Department of Health (DOH), and is working with the DOH and the Media School at the College of Santa Fe in developing educational awareness tools and materials.

Los Alamos County Annual Science Fair. David Kilcrease, T-4, served as an advisor on the board for the Los Alamos County Annual Science Fair.

Careers and Curiosity in Math and Science is a program designed to foster girls' interest in science and math. The program provides an interactive scientific experience, guided by women scientists and mathematicians and is offered to elementary-school-level children (boys and girls). The goals of the program are to stimulate interest in learning science and mathematics for teachers and students; to raise teacher awareness of gender equity issues relating to math and science education; to expose elementary students to career opportunities in science and mathematics; to foster self-esteem, ambition, and math and science interest in female students; and to provide positive female science and math role models. The project is jointly sponsored by the Laboratory, the American Association of University Women, and participating school districts. This program was co-originated by Denise George (T-1), who still plays an active role in organizing and participating in the program.

The annual Expanding Your Horizons Program is cosponsored by the Laboratory and is designed for young women in grades 8 through 10 from Northern New Mexico schools to provide a unique opportunity to explore careers in science, engineering, and mathematics. Each attendee participates in hands-on workshops and team-building activities conducted by women scientists and attends presentations and lectures regarding career opportunities in the science, engineering, and mathematics fields. The program encourages female students to take math and science courses in high school so as to not limit future career choices and offers examples of women who have successful scientific careers. Schools nominate students to participate in this daylong activity. T Division is one of the divisions sponsoring this program. Several female staff members in the Division have helped organize this event, presented workshops, and team activities. Tinka Gammel (T-1) is currently a committee member and presenter.

Appendix J (page 220) includes a list of staff who served as adjunct professors, on advisory committees, or as visiting scientists. These activities all contribute to our science education efforts.